

the rotational collision number ζ_{rot} by means of $(D_{rot})_1 / (D_{11})_1 = 1 - 1.22\zeta_{rot} - 2$. The ratio $\rho(D_{rot})_1 / (\mu)_1$ from the exact Mason-Monchick (1962) theory (where ρ is the d. and $(\mu)_1$, the viscosity coefficient) is nearly constant

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ACCESSION NUMBER: 1975:599798 CAPLUS
DOCUMENT NUMBER: 83:199798
TITLE: Rotational diffusion of linear molecules in fluids. Extended diffusion theory for perpendicular bands of linear molecules including vibrational relaxation
AUTHOR(S): Levi, G.; Marsault, J. P.; Marsault-Herail, F.; McClung, R. E. D.
CORPORATE SOURCE: Lab. Phys. Exp. Mol., Univ. Pierre et Marie Curie, Paris, Fr.
SOURCE: Journal of Chemical Physics (1975), 63(8), 3543-51
CODEN: JCPSA6; ISSN: 0021-9606
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Modifications are given of the classical and semiclassical extended diffusion theories, for the perpendicular bands of linear mols., wherein the collisional events which change the angular momentum of the mol. simultaneously bring about changes in the orientation of the transition moment vector. The ir band shapes for N2O and C2H2 in dense **gas** mixts. are in excellent agreement with the theor. band shapes.

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ACCESSION NUMBER: 1975:435140 CAPLUS
DOCUMENT NUMBER: 83:35140
TITLE: Rotational diffusion of nonassociated molecules in pure liquids and in dilute solutions
AUTHOR(S): Simova, P. D.; Kirov, N.
CORPORATE SOURCE: Inst. Solid State Phys., Sofia, Bulg.
SOURCE: Bulgarian Journal of Physics (1974), 1(1), 20-30
CODEN: BJPHD5; ISSN: 0323-9217
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In pure liqs. with elongated mols. the Brownian motion is highly anisotropic, and the preorientational potential barrier toward the short axis $U_{or}(\perp)$ is considerably higher than that toward the long axis, $U_{or}(.dblvert.)$. The difference between $U_{or}(\perp)$ and $U_{or}(.dblvert.)$ increases with the elongation of the mol. No spectral investigations prove any anisotropy of the Brownian motion. In dilute solns. of inert solvents (hydrocarbons) the rotational diffusion barriers of the same mols. with respect to the different axes are equal. This shows that the character of the mol. motion in pure liqs. and in solns. is different. In liqs. the intermol. interactions are stronger and the mols. are arranged rather rigidly with respect to their neighbors, so that great changes in the mol. orientation are unlikely and preorientation occurs only at small angles. This model can be a reasonably good approximation in the limiting cases when all mols. are trapped in potential boxes. In dilute, nonviscous solns. the rotational motion of the mols. consists of fast, **gas**-like orientation steps at large angles with crossing over the potential barrier: its height is determined by the viscosity of the solvent. In this case no preferred direction of the rotational diffusion is observed. The same results were obtained by W. Rotschild (1971), who investigated 1:4 solns. of CHCl3 in C6H6 and calculated the correlation function. The determination of U_{or} for the mols. in solns. is reliable only for nonassocd. systems. In associated systems, the effect of the Brownian motion on the half-width of the band becomes insignificant and other mechanisms of band broadening become important. Parameters are tabulated for 2-5 bands of PhCN and PhBr in solution in the n-paraffins C5-C15.

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L3	288 S ROTATION (W) DIFFUSION
L4	10 L3 AND (GALLIUM OR GA)